Liquid Chromatography/Mass Spectrometry Library Development and Strategy for Identifying Harmful Organics in Drinking Water

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The Homeland Security Presidential Directive (HSPD-9) mandates that the U.S. Environmental Protection Agency (U.S. EPA) Office of Water expand its monitoring and surveillance systems for recognizing a terrorist attack on, or other significant change to, water quality. This is a daunting task to undertake due to the vast breadth of chemical compounds and numerous water sources required to be monitored. Water is our most abundant and most important natural resource, so it is vital that we develop strategies to detect and react to harmful chemicals in our water supply.

In light of this issue, U.S. EPA Region 5 Central Regional Laboratory (CRL) is collaborating with Waters Corporation, under a Cooperative Research and Development Agreement (CRADA), to develop a quick and robust method that will detect specific harmful agricultural, industrial, and pharmaceutical compounds in drinking water. This method is based on developing a searchable mass spectral library system for liquid chromatography/mass spectrometry (LC/MS and LC/MS/MS) analysis. Many harmful organic compounds of interest, such as pesticides, pharmaceuticals, and drugs of abuse, are nonvolatile and therefore not amenable to gas chromatography/mass spectrometry (GC/MS), for which MS libraries are in widespread use. There are currently no transferable LC/MS libraries available for practical use.

Aside from GC/MS, there are LC methods using various detection systems available wherein chromatographic resolution is critical for identification and quantification. However, these LC non-MS methods are not well suited for the important task of screening for a large variety of potentially co-eluting harmful organic compounds in drinking water simultaneously. LC/MS is highly specific in that it can resolve molecular fragments down to a single m/z (mass/charge) unit. This specificity allows for detection of harmful organic compounds without the requirement of high chromatographic resolution. Therefore, if an LC/MS library system were to be developed, a water sample could be screened for selected harmful organics using a single, universal, reversed-phase gradient, thus saving time and money.